11:36

J13 2 Calculations of the Doping limits in ZnSe

DAVID LAKS, IBM Thomas J. Watson Research Center.

ZnSe and other wide-band-gap semiconductors have always been plagued by doping problems, particularly for p-type material. We use first-principles density-functional-theory calculations to provide a comprehensive description of the semiconductor-dopant system, using ZnSe doped with Li, Na, or N acceptors as our examples. Calculations are performed for the' native point defects, the dopant atoms at different sites in the crystal, and for the bulk solid phases of the native and dopant atoms. By introducing the chemical potentials of the various atomic species, we address the issues of (I) compensation by native defects and its relation to the stoichiometry of the host crystal, (2) self-compensation reactions in which substitutional acceptors become donors by moving to interstitial sites, and (3) the salubility of the acceptor dopants. Our results show that native-defect compensation and self-compensation can be avoided by adjusting the growth conditions, while acceptor solubility poses a much more serious limit to acceptor-doping of ZnSe.

This work was performed in collaboration with C. G. Van de Walle, G. F. Neumark, and S. T. Pantelides.